

4-(Chloromethyl)-2-ethoxy-1,3,2lambda⁵- dioxaphospholan-2-one

67554-11-4 | DTXSID50791173

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 201 °C

Global applicability domain: Inside

Local applicability domain index: 5.48e-01

Confidence level: 4.78e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dichlorvos</div> <div>Measured: 234</div> <div>Predicted: 221</div>	<div>Image not found</div> <div>Diethyl phosphorochloridate</div> <div>Measured: 93.5</div> <div>Predicted: 125</div>	<div>Image not found</div> <div>Cyclosarin</div> <div>Measured: 239</div> <div>Predicted: 216</div>
<div>Image not found</div> <div>Sulfurous acid, bis(2-methylpropyl) ester</div> <div>Measured: 210</div> <div>Predicted: 214</div>	<div>Image not found</div> <div>Phosphonic acid, vinyl-, diethyl ester</div> <div>Measured: 202</div> <div>Predicted: 205</div>	